Monte Carlo calculation of $In_{0.53}Ga_{0.47}As$ and InAs noise parameters

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***Abstract*—The increase of modern electronics performances depends on the ability to grow high-frequency, low-noise and low-power devices. Nowadays, InP technology is mature and $In_{0.53}Ga_{0.47}As$ is clearly a material of interest. Moreover, Sb-based devices constitute the next step [1], which makes InAs transport and noise parameters analysis a relevant topic.**

The difficulties to obtain these quantities through experiments can be overcome by the onset of an appropriate numerical protocol. In this framework, we propose a Monte Carlo calculation of both diffusion coefficient and noise temperature of bulk $In_{0.53}Ga_{0.47}As$ and InAs within a correlation functions formalism.

I. Introduction

Both InAs and $In_{0.53}Ga_{0.47}$ are among the most promising materials for low-power high-frequency applications with nano-scale electron devices. In this framework, the study of noise features show a multiple interest:

- firstly, the noise-to-signal ratio is a critical parameter which has to be extracted in order to evaluate the ability of a given compound to operate correctly;
- then, some parameters which characterize the bulk material, such as diffusion coefficient or thermal conductivity, are linked to its noise behavior;
- finally, the interpretation of the behavior of the noise parameters as functions of the frequency and bias conditions allow to make a kind of in-device spectroscopy which allow to emphasize the microscopic phenomena influencing the electron gas.

If noise investigations are not so trivial to be led in an experimental way, they are made possible within a theoretical approach, since the Monte Carlo simulation of charge transport naturally describes the stochastic aspect of electron motion [2]. The paper is organized as follows: in Section 2, the theoretical framework is given and the different calculated quantities are described. Then, in Section 3, the obtained results are presented and discussed. The conclusion is then given in Section 4.

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II. Theoretical framework

The charge transport in bulk $In_{0.53}Ga_{0.47}As$ and InAs is simulated at room temperature with a Monte Carlo procedure accounting for the electron dynamics [3], [4]. The conduction band is modeled with three spherical non-parabolic valleys. We consider collisions with ionized impurities (Brooks-Herring model), polar an non-polar optical phonons, acoustic phonons and intervalley phonons. The input data are calculated by interpolating the values of the corresponding binary materials [5], [6], [7], [8], [9]. Pauli exclusion principle is implemented through the standard algorithm [10].

The simulator has been previously validated by comparison with experimental data [11], [12], [6], and the results are in agreement with the simulations of Bude and Hesse [13]. Note that the first-order material parameters as well as their analytical interpolations have been published in reference [14].

The noise parameters are calculated through a correlation functions formalism. According to Wiener-Khintchine theorem, considering stationary conditions, the spectral density of the velocity fluctuations of a given carrier verifies the relation [15], [2]

$$S_v(f) = 4\int_0^\infty \cos(2\pi f\tau) C_{\delta v}(\tau)\, d\tau \tag{1}$$

where $C_{\delta v}(\tau)$ is the autocorrelation function of the velocity fluctuations $\delta v(t)$, which can be considered in any simulated directions, and which satisfies the relation

$$C_{\delta v}(\tau) = \overline{\delta v(t)\cdot \delta v(t+\tau)} \tag{2}$$

From these quantities, one can determine the diffusion coefficient D in both parallel and perpendicular directions (with respect to the electric field E direction). Indeed, it verifies the frequency relation

$$D(E,f) = \frac{1}{4} S_v(E,f) \tag{3}$$

so that D can be calculated for ohmic regime as well as for hot electron conditions. In static and ohmic conditions, the longitudinal and transverse diffusion coefficients constitute

the same quantity D_0, which is directly related to the ohmic mobility μ_0 by the Einstein relation

$$D_0 = \frac{K_B T}{q} \mu_0 \tag{4}$$

However, when we consider dynamic and/or far-for-equilibrium regimes, the previous relationship is broken and must be modified in order to make appear the differential mobility μ' and a generalization of the lattice temperature. This latter quantity, the noise temperature T_N, is then linked to the longitudinal part of the diffusion coefficient through a generalization of the Einstein relation [16]:

$$T_N(f,E) = \frac{D_{\|}(f,E) q}{K_B Re\{\mu'(f,E)\}} \tag{5}$$

III. Results

A. Correlation functions and spectral densities

We report in Fig. 1 the autocorrelation functions of velocity fluctuations $C_{\delta v}(t)$ as functions of time, calculated in the longitudinal direction for both InGaAs and InAs, and for different values of the applied electric field. Note that we

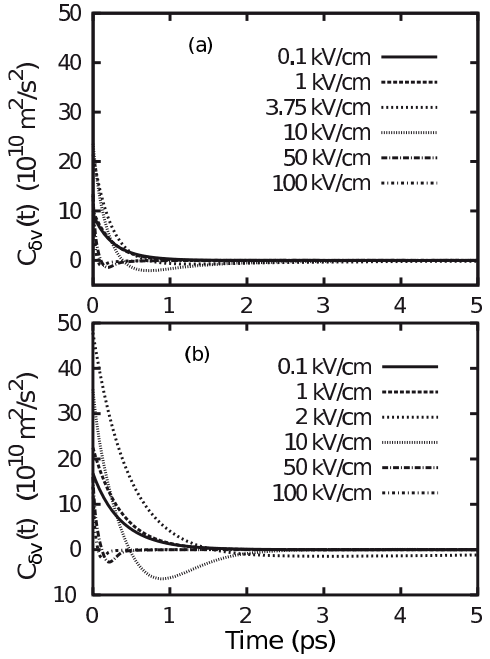

Fig. 1. Autocorrelation function of the longitudinal velocity fluctuations $C_{\delta v}(t)$ as a function of time for different electric fields for InGaAs (a), and InAs (b). We consider a doping concentration of $N_D = 10^{16}$ cm^{-3} at room temperature.

have considered a doping concentration of $N_D = 10^{16}$ cm^{-3} at room temperature. We observe that for low electric fields, when thermodynamic equilibrium is reached, the obtained autocorrelation function of velocity decays exponentially with a characteristic time related to the momentum relaxation. For sufficiently high electric fields, the autocorrelation functions exhibit negative values in both materials. This behavior can be attributed to the existence of two different relaxation times, one associated with the momentum relaxation processes, and the other to the energy relaxation ones. The negative part is more important, for a given electric field, in InAs that in InGaAs. We also observe that the auto-correlation functions tend faster to their zero values as the electric field increases: this is linked to the onset of phenomena associated with hot-carrier effects, that is for example optical phonon emission, which break the dynamics of the carriers in a relatively short time.

The corresponding spectral densities are reported in Fig. 2. In ohmic regime, the characteristic Lorentzian shape is ob-

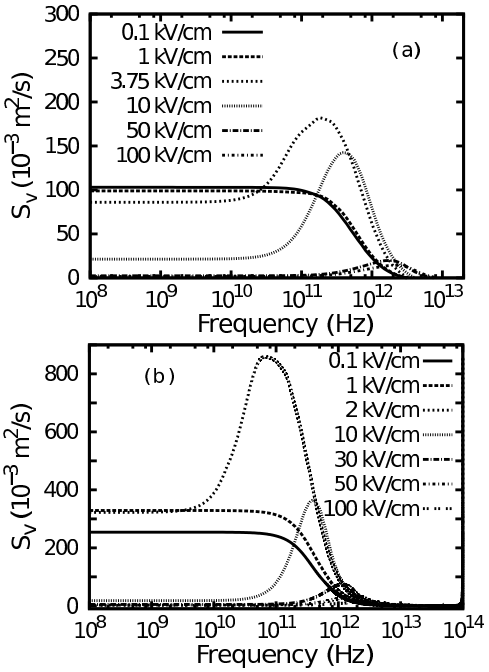

Fig. 2. Spectral densities of velocity fluctuations S_v as a function of frequency for different values of the electric field in InGaAs (a) and InAs (b).

served while, for the highest values of the electric field, a bump appears just before the cut-off frequency. Ranging between the GHz and THz frequency domains, this bump is directly related with the negative part of the autocorrelation function and then to the activation of high-energy collision processes. As concerns the plateau, it is directly linked to the static longitudinal diffusion coefficient, according to Eq. (3) with $f = 0$.

B. Longitudinal and transverse diffusion coefficients

Figure 3 reports the diffusion coefficient as a function of the electric field in longitudinal and transverse directions, for both InGaAs and InAs, in the conditions previously considered. For the case of InGaAs, comparisons with other theoretical results [17] show a quite good agreement, in particular for the case of the longitudinal coefficient. For the weakest values of the electric field, D is quite constant and the Einstein relation which links it to the ohmic mobility is verified. It then increases to reach its maximum value around the threshold field, for which the inter-valley transfer is activated, because of a stronger coupling between momentum and energy relaxation

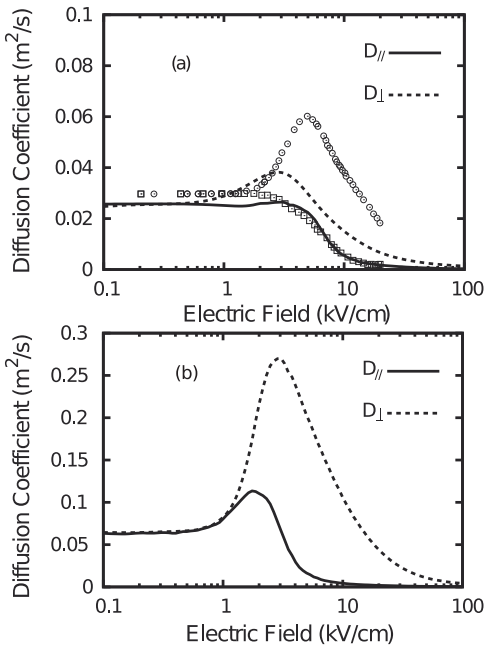

Fig. 3. Diffusion coefficient as a function of the electric field for InGaAs (a) and InAs (b) in both longitudinal and transverse directions (as compared with the applied electric field axis). Lines represents our MC simulations and symbols the theoretical results of Bourel *et al.* [17].

processes. This effect is more important in the transverse direction than in the longitudinal one, which is related to the anisotropy of the onset collisions. Finally, we observe, as expected, that the diffusion coefficient is higher in InAs than in InGaAs, which is linked to a better mobility.

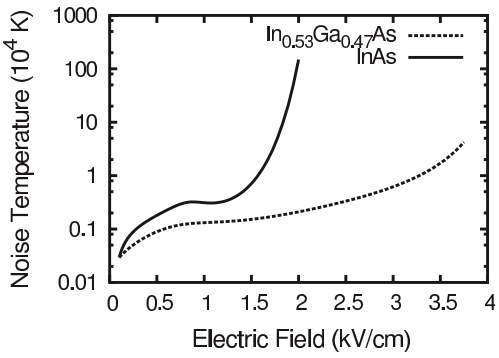

Fig. 4. Noise temperature as a function of electric field for bulk $In_{0.53}Ga_{0.47}As$ and InAs at room temperature and with a donor concentration $N_D = 10^{16}$ cm^{-3}.

C. Noise temperature

Considering the obtained results for the longitudinal diffusion coefficient and Eq. (5), we have calculated the noise temperature T_N in the considered materials in static conditions, and reported them as functions of the electric field in Fig.4. Obviously, for low electric fields, the noise temperature is found to be equal to the lattice temperature. However, T_N increases with the electric field, since the reduction in differential mobility becomes important as compared to the variations of the diffusion coefficient. For all the considered electric fields, we observe that the noise temperature is always greater in InAs that in InGaAs, according to the greater mobility of the former. For both materials, the noise temperature diverges as the electric field approaches a threshold value, which is higher in InGaAs that in InAs. The threshold field corresponds to the decrease of the drift velocity which is associated with the negative differential mobility of III-V materials. This behavior of the noise temperature indicates the appearance of an electric instability, namely the Gunn effect due to the inter-valley transfers in the considered materials.

IV. Conclusion

We have calculated the noise parameters of $In_{0.53}Ga_{0.47}As$ and InAs bulk materials at room temperature within a Monte Carlo approach and a correlation functions formalism. A special interest was given to the velocity fluctuation autocorrelation functions and their spectral densities, the diffusion coefficient in both longitudinal and transverse directions, and to the noise temperature. The obtained results emphasize the microscopic effects which are involved in the different bias conditions. In particular, a strong influence of hot electron transport on the diffusion coefficient on one hand, and of the internally transfer on the noise temperature on the other hand, were reported.

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